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**OPTIMAL DESIGN PROCEDURES FOR TWO-LEVEL FRACTIONAL
FACTORIAL EXPERIMENTS GIVEN PARTIAL PRIOR
INFORMATION ABOUT PARAMETERS**

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TECHNICAL PAPER proposed for presentation at 131st Annual
Meeting of the American Statistical Association in Conjunction
with the Allied Social Science Associations
Fort Collins, Colorado, August 23-26, 1971

OPTIMAL DESIGN PROCEDURES FOR TWO-LEVEL FRACTIONAL FACTORIAL
EXPERIMENTS GIVEN PARTIAL PRIOR INFORMATION ABOUT PARAMETERS

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ABSTRACT

Any prior information an experimenter has should be incorporated into the design of further experiments. Assume such information is expressed as probabilities that each parameter of the full factorial model is nonzero. This report develops optimal design procedures by posing the experimental design problem as a finite decision problem. Bayes and mini-max design strategies are then derived and their application illustrated. The major computational step is the evaluation of all possible matchings of physical variables to the abstract variables of all potential designs. The technique of telescoping sequences of blocks permits the consideration of experiments to be performed in stages.

SYMBOLS

B	complete set of parameters or coefficients
$B(h)$	subgroup of B used at the h^{th} stopping point of experiment
h	denotes the stopping point of the experiment
$S(i,h)$	the set of standard order subscripts of the elements of $\beta_i \otimes B(h)$
n	number of factors or independent variables
n_h	number of treatment combinations at the h^{th} stopping point
p_b	prior probability of a block effect not being zero
p_i	prior probability that $\beta_i \neq 0$
p_{hs}	probability the experiment terminates at exactly the h^{th} stopping point
U	total expected utility for a given strategy
$U(h)$	total expected utility of the h^{th} stopping point for a given strategy

$U(i,k)$	expected utility gained by assigning the estimator for $\beta_i \otimes B(h)$ to β_k
$U(i,b)$	expected utility gained by assigning the estimator for $\beta_i \otimes B(h)$ to the block effect that alias set is confounded with
$u_i(h)$	utility assigned to an unbiased estimate of β_i at the h_{th} stopping point of the experiment
X_A, X_B, \dots	independent variables (design)
X_0, X_I	dummy independent variables which are identically equal to one for all treatment combinations
X_i	independent variables (physical) $i = 1, 2, \dots, n$
\otimes	a group operation
Y	random response or dependent variable
y	observed value of Y
β_A, β_B, \dots	parameters of a model equation in the design variables
β_1, β_2, \dots	parameters of a model equation in the physical variables
β_0, β_I	constant terms of the model equation
b_1, \dots	estimates of the parameters β_1, \dots
b_A, \dots	estimates of the parameters β_A, \dots
$\beta_i \otimes B(h)$	coset obtained by multiplying all elements of $B(h)$ by β_i
δ	random error

INTRODUCTION

In a two-level full factorial experiment with n independent variables X_A, X_B, \dots there are 2^n possible distinct treatment combinations. If all the treatment combinations are performed, it is possible to estimate the β 's in the model equation of the form

$$\begin{aligned}
Y = & \beta_I + \beta_A X_A + \beta_B X_B + \beta_{AB} X_A X_B + \beta_C X_C \\
& + \beta_{AC} X_A X_C + \beta_{BC} X_B X_C + \beta_{ABC} X_A X_B X_C + \dots \\
& + \beta_{ABC\dots} X_A X_B X_C \dots + \delta
\end{aligned} \tag{1}$$

where δ is a random variable with mean zero and finite variance.

It will be convenient at this point to introduce an alternate notation for equation (1). Let the n independent variables be denoted as X_1, \dots, X_n . Number the 2^n β 's in equation (1) from β_0 to β_{2^n-1} and consider the following equation similar to equation (1).

$$\begin{aligned}
Y = & \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \beta_3 X_1 X_2 + \beta_4 X_3 + \\
& + \dots + \beta_{2^n-1} X_1 X_2 \dots X_n + \delta
\end{aligned} \tag{2}$$

Equation (1) and equation (2) are both written in what is called the standard order. If the subscripts of the β 's are rewritten as n -digit binary numbers, it becomes quite obvious how the terms and coefficients of equation (2) are related to their standard order number. For example, let $n = 4$ and consider the following equation where the subscripts on the β 's are written as binary numbers.

$$\begin{aligned}
Y = & \beta_0 + \beta_1 X_1 + \beta_{10} X_2 + \beta_{11} X_2 X_1 \\
& + \beta_{100} X_3 + \beta_{101} X_3 X_1 + \beta_{110} X_3 X_2 \\
& + \beta_{111} X_3 X_2 X_1 + \beta_{1000} X_4 + \beta_{1001} X_4 X_1 \\
& + \beta_{1010} X_4 X_2 + \beta_{1011} X_4 X_2 X_1 + \beta_{1100} X_4 X_3 \\
& + \beta_{1101} X_4 X_3 X_1 + \beta_{1110} X_4 X_3 X_2 + \beta_{1111} X_4 X_3 X_2 X_1
\end{aligned} \tag{3}$$

In general a β whose subscript in binary notation has ones in the i_1, i_2, \dots, i_k locations from the right is the coefficient of the $X_{i_1} X_{i_2} \dots X_{i_k}$ interaction.

It is well known that the set of all 2^n coefficients or parameters form a group denoted B under the appropriate operation denoted \otimes . In the alphabetic notation this operation is simply commutative multiplication of the letters with the exponents reduced modulo 2. In the binary type notation this operation may also be denoted \otimes and is defined as

$$\beta_m \otimes \beta_k = \beta_{m_n m_{n-1} \dots m_1 \otimes k_n k_{n-1} \dots k_1}$$

$$= \beta_{d_n d_{n-1} \dots d_1}$$

where $d_i = (k_i + m_i) \pmod{2}$.

Thus for example

$$\beta_{CBA} \otimes \beta_{DCB} = \beta_{DC^2 B^2 A} = \beta_{DA}$$

and

$$\beta_{0111} \otimes \beta_{1110} = \beta_{1001}.$$

A regular fractional replicate of the full factorial design does not allow separate estimation of all of the β 's. Certain linear combinations of them can be estimated however. The aliased sets of parameters which can be estimated depends upon the treatment combinations composing the fractional replicate, or equivalently upon the choice of the defining parameter group (d.p.g.)

Holms and Sidik (ref. 1) present a discussion of double (and multiple) telescoping sequences of blocks. Telescoping allows an experimenter to perform a factorial experiment in stages where the starting stage is a small regular fractional replicate and the final stage is some larger regular fraction. Each succeeding stage adds treatment combinations to those already performed in earlier stages. In order to retain orthogonality and orthogonal blocking each stage must be a power of two times the size of the preceding stage and all the treatments run must themselves form a regular fraction. This requirement implies that the d.p.g. defining the regular fraction at any stage must be a subgroup of the d.p.g. of the previous stage. Since multiple telescoping allows several possible choices of subgroups from each preceding group and each such choice may correspond to a potential stopping point we will simply index the stopping points by h and ignore the relations among the groups. Thus the d.p.g.'s that define fractional replicates at the stopping points are subgroups $B(h)$ of B . The aliased sets of parameters at each stopping point are the cosets $\beta_i \otimes B(h)$.

At this point a distinction between physical and design variables will be made. The physical variables in an experiment will be denoted as X_1, X_2, \dots, X_n . Each X_i is chosen to represent one of the physical variables and is fixed for the remainder of the experiment. For example

X_1 = temperature

X_2 = time

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· ·

· ·

X_n = velocity

The design variables will be denoted as X_A, X_B, X_C, \dots and so forth. These variables represent abstractions and tables exist (for example, the NBS tables (ref. 2) or Addelman's tables (ref. 3)) which tabulate experimental designs in terms of these design variables. When an experimenter consults one of these tables and chooses a design, he must then determine a matching of the design variables and the physical variables. Ordinarily the choice is arbitrary because the experimenter is not assumed to have any prior information available which would indicate one matching might be preferred to another. We consider the problem of choosing a best design under the following conditions of prior knowledge:

1. For each β_i the experimenter can specify $p_i = P\{\beta_i \neq 0\}$.
2. For each β_i and each h denoting a possible stopping point of the experiment the experimenter can specify the value to him of obtaining an unbiased estimate of β_i . This is denoted by $u_i(h)$.
3. For each h denoting a possible stopping point of the telescoping experiment the experimenter can specify p_{sh} = probability of stopping exactly at the h^{th} stopping point.

Recall that none of the β 's may be separately estimated from a fractional factorial experiment unless some assumptions about certain others of the β 's are introduced. Conditions one and two above provide assumptions that will enable the experimenter to assign the estimator for an alias set to a single parameter from the alias set and evaluate the consequences of this.

It is also evident that changing the matching of design and physical variables will change the alias sets. For if the matching for $n = 4$ is

$$X_1 = X_A$$

$$X_2 = X_B$$

$$X_3 = X_C$$

$$X_4 = X_D$$

(4)

then the alias set $\{\beta_A, \beta_B, \beta_{DBA}, \beta_D\}$ is mapped into $\{\beta_{0001}, \beta_{0010}, \beta_{1011}, \beta_{1000}\} = \{\beta_1, \beta_2, \beta_{11}, \beta_8\}$. But the matching

$$X_1 = X_B$$

$$X_2 = X_A$$

$$X_3 = X_D$$

$$X_4 = X_C$$

(5)

maps $\{\beta_A, \beta_B, \beta_{DBA}, \beta_D\}$ into $\{\beta_{0010}, \beta_{0001}, \beta_{0111}, \beta_{0100}\} = \{\beta_2, \beta_1, \beta_7, \beta_4\}$

The steps of the design and performance of the experiment may now be represented as a finite discrete game between the experimenter and nature. The decision space E for the experimenter is composed of the choice of initial defining parameter group, choice of sequence(s) of subgroups that define the telescoping, choice of physical-design variable matching, and the choice of parameter-estimator matching. The decision space N for nature consists of the choice of which of the β 's will be nonzero and the choice of the stopping point of the experiment.

A flow diagram is presented in fig. 1 which indicates the sequence of choices to be made by the experimenter and nature.

It should be noted that the order of presentation shown in fig. 1 of the choices of nature and the experimenter are not necessarily in temporal order. The choice of d.p.g. and physical-design variable matching are interchangeable but must be made before the actual execution of the experiment. Nature's choice of the parameter values would normally be considered to be made prior to anything the experimenter does. However, it does no harm to conceive of nature being permitted to choose the parameter values after the experiment is performed. In fact, this concept is more convenient in describing the Bayes decision procedure for the experimenter.

Once given the structure of a game or a decision problem and the utilities of the outcomes, the statistician must devise a method for choosing among the possible alternatives (i.e., choose a strategy) so that a desirable outcome is finally attained.

There are two general principles by which strategies are ordered which are in current use. One is the Bayes principle and the other is the mini-max principle.

The Bayes Solution

The Bayes procedure assumes that nature is an indifferent participant in the game. Thus, the choices that nature makes are independent of the choices available to the experimenter but instead are made according to a specified probability distribution. Any information the experimenter may have concerning the strategy (i.e., the specified probability distribution) nature will follow is useful information that should be incorporated into the decision procedure. The strategy for the experimenter which maximizes the utility, given the assumed strategy for nature, is the Bayes strategy.

Before considering how best to match physical and design variables let us assume that some matching has been made. Then consider the problem of matching estimators and parameters at the h^{th} stopping point. The d.p.g. is $B(h)$ and the alias sets are all those distinct cosets of the form

$$\beta_i \otimes B(h) = \{\beta_{i_1}, \beta_{i_2}, \dots, \beta_{i_m}\} \quad (6)$$

If the parameter $\beta_k \in \beta_i \otimes B(h)$ and the estimator for that alias set is assigned to β_k , then, assuming independence, the prior probability that the estimator will be unbiased is

$$\prod_{\substack{j \in S(i,h) \\ j \neq k}} (1 - p_j) \quad (7)$$

Since $u_i(h)$ is the utility of an unbiased estimate of β_i at the h^{th} stopping point

$$U(i,k) = u_k(h) \prod_{\substack{j \in S(i,h) \\ j \neq k}} (1 - p_j) \quad (8)$$

is the expected utility of the decision to assign the estimator for the alias set $\beta_i \otimes B(h)$ to the parameter β_k . Thus the Bayes strategy is to assign the estimator to the parameter of the alias set which maximizes this expected utility. A special case requires separate discussion. Suppose that an alias set is confounded with some block effect. Assume that prior probabilities can be assigned to the event that each block effect will be nonzero and assume the utility of an unbiased estimate of each block effect can be specified. Then this information can be incorporated into the decision procedure by computing the two expected utilities.

$$U(i,k) = u_k(h) \prod_{\substack{j \in S(i,h) \\ j \neq k}} (1 - p_j) (1 - p_b) \quad (9)$$

$$U(i,b) = u_b \prod_{j \in S(i,h)} (1 - p_j) \quad (10)$$

where $p_b = P \{ \text{the block effect} \neq 0 \}$

u_b = utility of an unbiased estimate of the block effect and

$U(i,b)$ = the expected utility gained by assigning the estimator for $\beta_1 \otimes B(h)$ to the block effect.

Normally one would expect $u_b = 0$ and hence $U(i,b) = 0$ thus not necessitating the calculation in equation (10).

In connection with block effects it is also important to note that depending upon how the block parameters are defined, the estimator for the d.p.g. may be confounded with blocks.

Since the alias sets are disjoint and the estimators for each alias set are independent of each other, it follows that the choice of parameter from one alias set should not influence the choice from another alias set. Thus for the chosen matching of physical and design variables, the chosen defining contrasts, and the chosen estimator-parameter matching, the expected utility at the h stage may be denoted

$$U(h) = \sum U(i, k_{\max}) \quad (11)$$

where the summation is over all the distinct cosets at the h^{th} stage, and k_{\max} is the choice of k within each coset which maximizes $U(i,k)$. By condition 3 on page 5 it is also assumed that the experimenter can specify the probabilities of stopping exactly at each of the stopping points. Thus,

$$U = \sum_h p_{sh} U(h) \quad (12)$$

represents the total expected utility over all the stages given the choice of the defining parameter groups and physical-design variable matching.

The formal Bayes procedure is then to compute U for all possible distinct choices of d.p.g.'s and physical-design variable matchings and use any choice which gives the maximum U .

Mini-Max Solution

To derive a mini-max strategy, the statistician assumes nature to be an aggressive player who will choose alternatives available which will minimize the maximum utility the statistician may gain. Thus the experimenter is the maximizing player and nature is the minimizing player.

A strategy for nature involves two component choices: the choice of which parameters will be nonzero and the choice of the path and stopping point of the telescoping. One choice available to nature which the experimenter has no influence upon is the choice of nonzero parameters. In fact, it is possible that nature may choose to let every parameter be nonzero. In this instance it will not be possible to obtain unbiased estimates for any parameter until the full replicate is run. If the utility function is restricted to be zero when the estimator is biased, then there is zero utility except for the full replicate. Thus, the only possible way for the experimenter to obtain a gain is to design for the full replicate. However, nature also may choose the stopping stage and so to minimize the experimenter's utility, any stage other than the full replicate may be chosen giving a utility of zero. Thus, any strategy at all that the experimenter uses will be a mini-max strategy.

Two less aggressive strategies for nature are conceivable. The first assumes that nature will still choose to have every parameter nonzero but will stop the experiment at one of the stages according to prior probabilities known by the experimenter. Then the only reasonable approach for the experimenter is to choose a design which maximizes the utility of the full factorial. Clearly this only involves minimizing losses due to block confounding.

The second of these less aggressive strategies allows that nature will choose the parameters to be nonzero according to probabilities known to the experimenter but will choose the stopping stage so as to minimize the experimenter's maximum utility. To find the mini-max strategy, the tree form of the game can be reduced to the form of a rectangular game and the technique of linear programming applied to determine the optimal strategies. Considering the size of the tree in many problems it does not seem likely that this approach would be computationally feasible.

Assignment of Utility Functions

The utility function is a function defined upon the space of all possible outcomes of a decision problem. This function describes the absolute or relative value to the decision maker of each of these outcomes. Methods of specifying the utility function based upon the axioms of utility theory are given in Raiffa (ref. 4) and DeGroot (ref. 5). These methods involve choices of lotteries and would be extremely impractical and cumbersome for most problems. Instead, the following five utility functions are offered as being both practical and somewhat representative of the decision makers preferences in the appropriate instances.

$$1. \quad u_i(h) = \begin{cases} 1 & \text{if estimator unbiased} \\ 0 & \text{if not} \end{cases} \quad (13)$$

This is a utility function which simplifies the expected utility to be the probability of getting an unbiased estimate of the parameter. This might be a useful utility function in the more basic scientific exploration where relative evaluations of the importance of specific parameters are not possible.

$$2. \quad u_i(h) = \begin{cases} p_i & \text{if unbiased} \\ 0 & \text{if biased} \end{cases} \quad (14)$$

This simple utility function can be thought of as representing the prior probability that an estimator will be unbiasedly estimating a nonzero quantity. Such a utility function might be used in response surface or optimum seeking experiments. This is true because a zero parameter contributes nothing toward being able to change the response by changing the levels of the independent variables.

$$3. \quad u_i(h) = \begin{cases} \sqrt{n_h} & \text{if unbiased} \\ 0 & \text{if biased} \end{cases} \quad (15)$$

where n_h = the number of treatment combinations at the h^{th} stopping point. This utility function could be useful in the situation where the experimental error is large and the cost of many observations is not much more than the cost of a few observations. The rationale for this is that the variance of an estimator is proportional to the inverse of the number of observations. Thus, one way to weight the value of an unbiased estimate is to weight it proportionately to the inverse of the standard deviation, that is, to $\sqrt{n_h}$.

$$4. \quad u_i(h) = \begin{cases} \frac{1}{n_h} & \text{if unbiased} \\ 0 & \text{if biased} \end{cases} \quad (16)$$

In the opposite situation to (3), suppose the experimental error is negligible but the cost of each observation is large so that the cost of the stage is a first degree function of the number of treatments. Then this utility function would weight the estimators more heavily at the early stages of the design and penalize the later stages.

$$5. \quad u_i(h) = \begin{cases} \frac{1}{\sqrt{n_h}} & \text{if unbiased} \\ 0 & \text{if biased} \end{cases} \quad (17)$$

This is an elementary combination of functions (3) and (4) and is intended for situations where both the costs of the observations are large and the experimental error is large.

Furthermore, a utility function might consist of a combination of (1) or (2) along with one of (3), (4), or (5).

CONCLUDING REMARKS

The two-level fractional factorial designs represent a class of designs of experiments yielding a large number of estimates of first-degree effects

and interactions for a small amount of experimentation. The main disadvantage of this class of designs is that the estimates are always estimates of aliased combinations of parameters. To make conclusions about single parameters it is necessary to have some information about the parameters from a source other than the experiment. If such information is available before the experiment is performed, it may be incorporated into the design of the experiment.

There are many situations in practice in which an experimenter may have varying amounts of information concerning the variables he wishes to investigate. This paper has developed some optimal design procedures when the prior information is:

1. For each parameter the experimenter states his prior probability that it is not zero, and

2. For each parameter the experimenter states what it is worth to him to obtain an unbiased estimate of it.

The information and decisions were formulated as a finite decision problem and Bayes and mini-max procedures were developed.

The main components of the problem were (1) the choice of estimator-parameter matching, (2) choice of physical-design variable matching, and (3) evaluations of all possible defining parameter groups and sequences of subgroups.

Modified Bayes and mini-max procedures which are computationally feasible were developed and some potential utility functions were presented.

The procedures presented here (described more fully in ref. 6) should prove to be of considerable value in application since the information required is of a nature that is easily specified and the computations required although tedious are amenable to being programmed for a digital computer. In fact, a computer program called NAMER (ref. 7) has been written and documented which determines the Bayes physical-design variable matching and the Bayes parameter-estimator matchings for a specified choice of d.p.g.'s at each stopping point of the experiment. Anyone wishing more information may write the authors at NASA Lewis Research Center, 21000 Brookpark Road, Cleveland, Ohio 44135.

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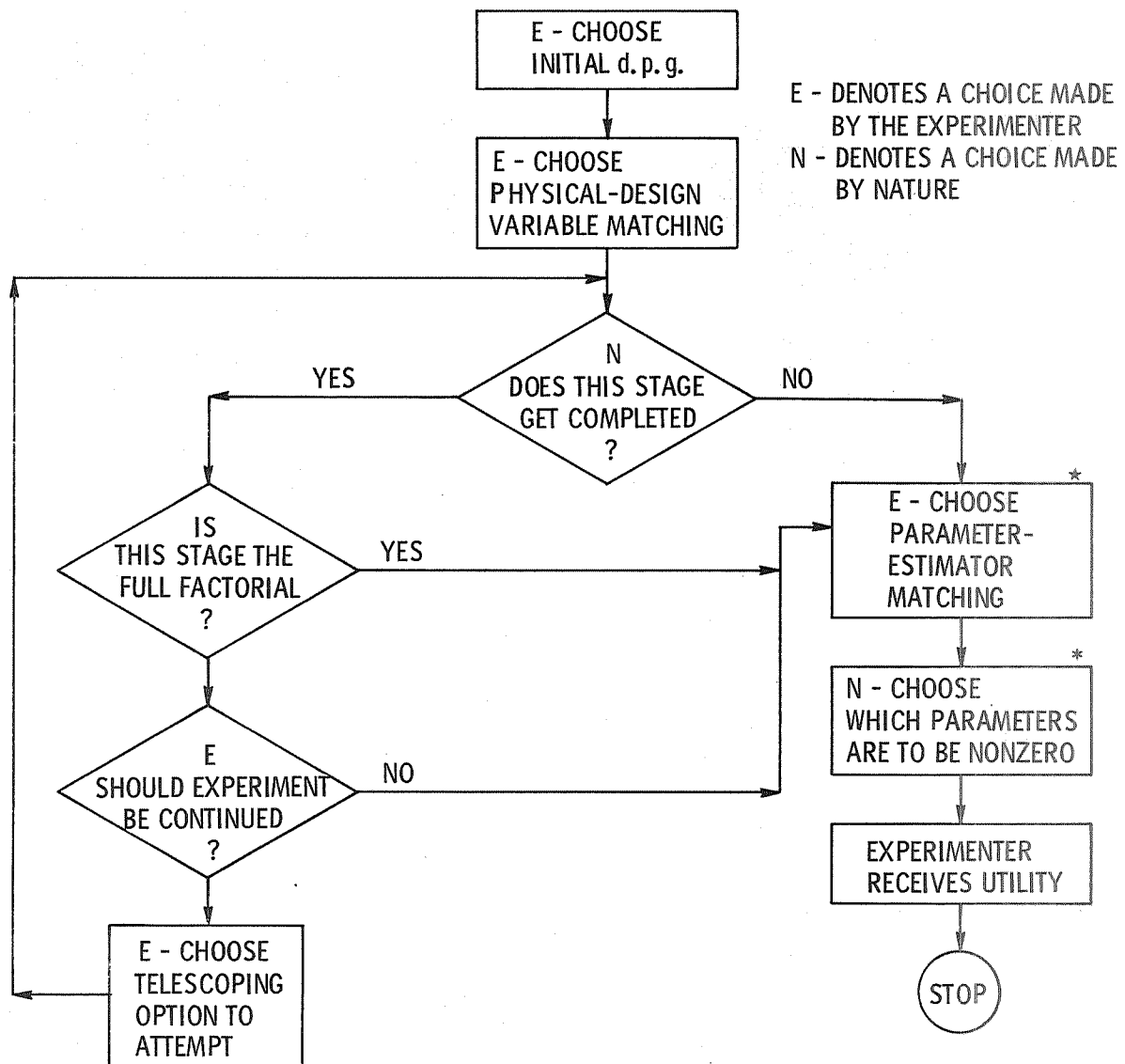


Figure 1. - Flow chart representing the sequence of choices made by the experimenter and nature.